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NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 4	DEC 18	CA/CAplus patent kind codes updated
NEWS 5	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 6	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS 7	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS 8	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 9	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 10	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 11	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 12	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 13	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 14	JAN 29	PHAR reloaded with new search and display fields
NEWS 15	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 16	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 17	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 18	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 19	FEB 26	MEDLINE reloaded with enhancements
NEWS 20	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 21	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 22	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 23	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 24	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 25	MAR 16	CASREACT coverage extended
NEWS 26	MAR 20	MARPAT now updated daily

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:45:45 ON 20 MAR 2007

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'REGISTRY' ENTERED AT 14:45:58 ON 20 MAR 2007
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DICTIONARY FILE UPDATES:  19 MAR 2007  HIGHEST RN 927525-36-8

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http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10538395-cl-46-47.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR
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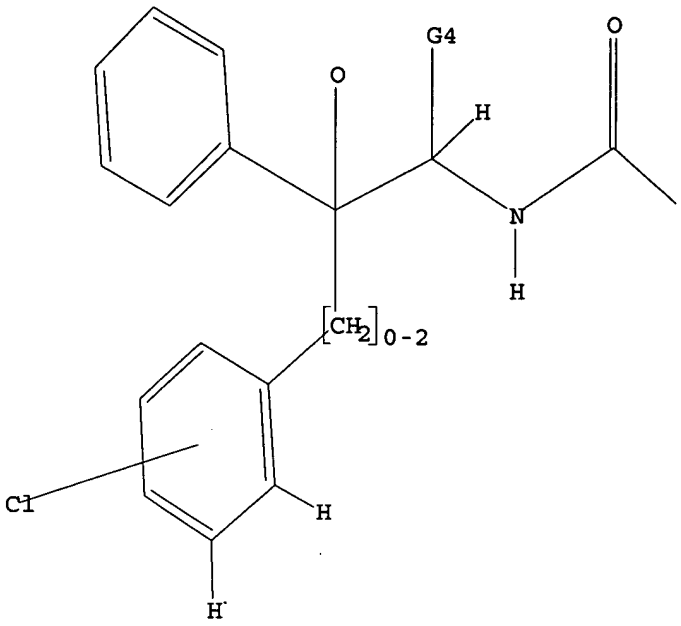

G1 Cy,Ak

G2 H,Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G3 H,Cy,Ak

G4 Me,Et

Structure attributes must be viewed using STN Express query preparation.

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=> s l1
SAMPLE SEARCH INITIATED 14:46:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       33 TO ITERATE

100.0% PROCESSED       33 ITERATIONS                                1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          316 TO     1004
PROJECTED ANSWERS:               1 TO       80

L2            1 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 14:46:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      567 TO ITERATE

100.0% PROCESSED      567 ITERATIONS                                8 ANSWERS
SEARCH TIME: 00.00.01

L3            8 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     172.10     172.31

FILE 'CAPLUS' ENTERED AT 14:46:34 ON 20 MAR 2007
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FILE COVERS 1907 - 20 Mar 2007 VOL 146 ISS 13
FILE LAST UPDATED: 19 Mar 2007 (20070319/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3
L4 1 L3

=> d l4

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:565042 CAPLUS
DN 141:106274
TI Preparation of substituted arylamides as cannabinoid-1 receptor antagonists
IN Lin, Linus S.; Hagmann, William K.; Kumar, Sanjeev; Yin, Wenji; Doss, George
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004058145	A2	20040715	WO 2003-US40040	20031215
	WO 2004058145	A3	20040902		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2510785	A1	20040715	CA 2003-2510785	20031215
	AU 2003300967	A1	20040722	AU 2003-300967	20031215
	EP 1575901	A2	20050921	EP 2003-814048	20031215
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	CN 1747926	A	20060315	CN 2003-80109750	20031215
	JP 2006510716	T	20060330	JP 2004-563615	20031215
	US 2006106071	A1	20060518	US 2005-538395	20050609
	IN 2005DN02542	A	20070119	IN 2005-DN2542	20050613
PRAI	US 2002-435436P	P	20021219		

WO 2003-US40040 W 20031215
OS MARPAT 141:106274

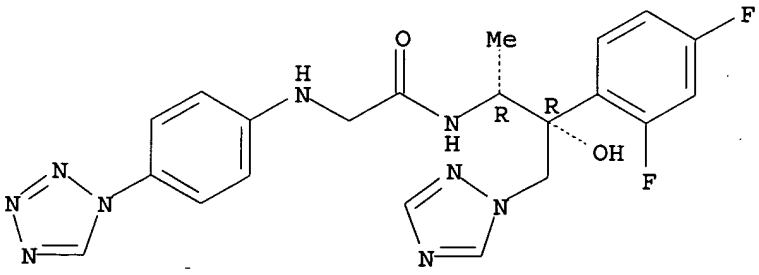
L19 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:658739 CAPLUS
DOCUMENT NUMBER: 136:5946
TITLE: Optically active antifungal azoles. XIII. Synthesis of stereoisomers and metabolites of 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-(1H-1-tetrazolyl)phenyl]-2-imidazolidinone (TAK-456)
AUTHOR(S): Ichikawa, Takashi; Yamada, Masami; Yamaguchi, Masashi; Kitazaki, Tomoyuki; Matsushita, Yoshihiro; Higashikawa, Keiko; Itoh, Katsumi
CORPORATE SOURCE: Medicinal Chemistry Research Laboratories I, Pharmaceutical Research Division, Takeda Chemical Industries, Ltd., Osaka, 532-8686, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2001), 49(9), 1110-1119
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:5946

AB The title imidazolidinone (I) is a new antifungal agent selected as a candidate for clin. trials. The three stereoisomers (1S,2R)-I, (1S,2S)-I and (1R,2S)-I were prepared as authentic samples to determine the enantiomeric and diastereomeric purity of I as well as to compare their in vitro antifungal activity. Pharmacokinetic studies of I using rats identified the existence of metabolites in the liver homogenate. The structures of the major metabolites were assigned as C-4 hydroxylated and/or C-5 hydroxylated 2-imidazolidinone derivs. based on HPLC and LC/MS/MS analyses. These hydroxylated compds. were prepared by reduction of the corresponding imidazolidinediones and confirmed to be identical to the metabolites by HPLC. In vitro antifungal activities of the three stereoisomers and the synthesized metabolites were considerably weaker than I.

IT 377079-03-3P 377079-07-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(multi-step preparation of antifungal (triazolylpropyl)(tetrazolylphenyl)imidazolidinone stereoisomers and their hydroxylated metabolites)

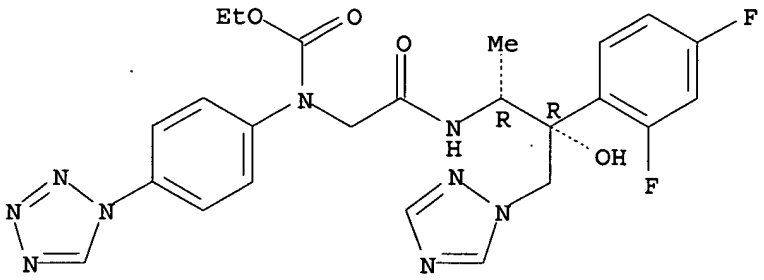
RN 377079-03-3 CAPLUS
CN Acetamide, N-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-2-[[4-(1H-tetrazol-1-yl)phenyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 377079-07-7 CAPLUS
CN Carbamic acid, [2-[[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]amino]-2-oxoethyl][4-(1H-tetrazol-1-yl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:384696 CAPLUS
DOCUMENT NUMBER: 133:173946
TITLE: A Three-Dimensional Model of Lanosterol 14α-Demethylase of Candida albicans and Its Interaction with Azole Antifungals
AUTHOR(S): Ji, Haitao; Zhang, Wannian; Zhou, Youjun; Zhang, Min; Zhu, Jie; Song, Yunlong; Lue, Jiaguo; Zhu, Jue
CORPORATE SOURCE: School of Pharmacy, Second Military Medical University, Shanghai, 200433, Peop. Rep. China
SOURCE: Journal of Medicinal Chemistry (2000), 43(13), 2493-2505
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The three-dimensional structure of lanosterol 14α-demethylase (P 45014DM, CYP51) of Candida albicans was modeled on the basis of crystallog. coordinates of four prokaryotic P450s: P450BM3, P450cam, P450terp, and P450eryF. The P 45014DM sequence was aligned to those of known proteins using a knowledge-based alignment method. The main chain coordinates of the core regions were transferred directly from the corresponding coordinates of P450BM3. The side chain conformations of the core regions were determined by the conformations of the equivalent residues with the highest homologous scores in four crystal structures. The model was then refined using mol. mechanics and mol. dynamics. The reliability of the resulting model was assessed by Ramachandran plots, Profile-3D, hydropathy plot anal., and by analyzing the consistency of the model with the exptl. data. The structurally and functionally important residues such as the heme binding residues, the residues interacting with redox-partner protein and/or involved in electron transfer, the residues lining substrate access channel, and the substrate binding residues were identified from the model. These residues are candidates for further site-directed mutagenesis and site-specific anti-peptide antibody binding expts. The active analog approach was employed to search the pharmacophoric conformations for 14 azole antifungals. The resulting bioactive conformations were docked into the active site of lanosterol 14α-demethylase of Candida albicans. All 14 azole antifungals are shown to have a similar docking mode in the active site. The halogenated Ph group of azole inhibitors is deep in the same hydrophobic binding cleft as the 17-alkyl chain of substrate. The π-π stacking interaction might exist between halogenated Ph ring of inhibitors and the aromatic ring of residue Y132. The long side chains of some inhibitors such as itraconazole and ketoconazole surpass the active site and interact with the residues in the substrate access channel. To

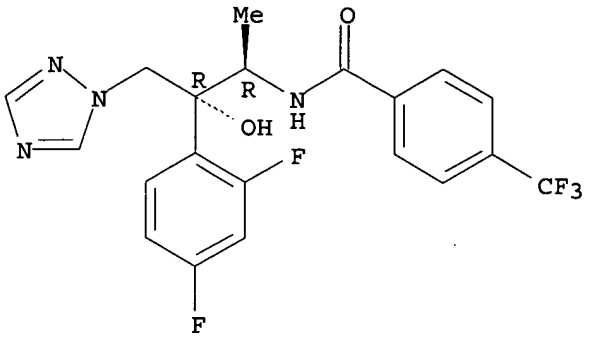
compare with mammalian enzymes, structurally selective residues of the active site of fungal lanosterol 14α-demethylase are distributed in the C terminus of F helix, β6-1 sheet and β6-2 sheet.

IT 136926-13-1
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(docking; three-dimensional model of lanosterol 14α-demethylase of Candida albicans and its interaction with azole antifungals)

RN 136926-13-1 CAPLUS

CN Benzamide, N-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:356189 CAPLUS

DOCUMENT NUMBER: 131:223005

TITLE: Pharmacophoric conformations of azole antifungals and their interaction with active site of target enzyme

AUTHOR(S): Ji, Haitao; Zhang, Wannian; Zhou, Youjun; Zhu, Jie; Zhu, Ju; Lu, Jiaguo

CORPORATE SOURCE: School of Pharmacy, Second Military Medical University, Shanghai, 200433, Peop. Rep. China

SOURCE: Yaoxue Xuebao (1999), 34(4), 280-285
CODEN: YHHPAL; ISSN: 0513-4870

PUBLISHER: Yaoxue Xuebao Bianjibu

DOCUMENT TYPE: Journal

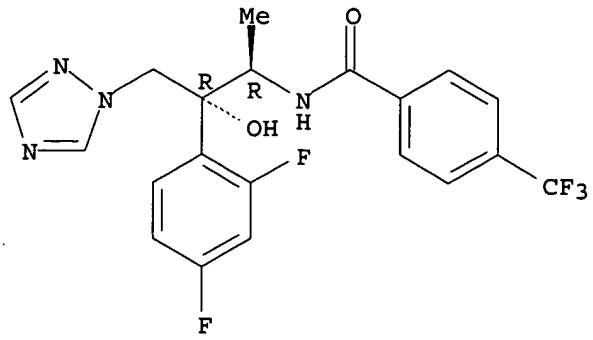
LANGUAGE: Chinese

AB The interactive mechanism of azole antifungals and functional residues of the active site of lanosterol 14α-demethylase of Candida albicans were studied. The global min.-energy conformations of 15 azole antifungals were determined by random conformation search and mol. dynamics simulated annealing, and the pharmacophoric conformations of the compds. were determined by active analog approach. All 15 azole antifungals had similar docking position in the active site, the structurally selective residues of the active site of fungal lanosterol 14α-demethylase were distributed in C terminus of F helix, β6-1 sheet and β6-2 sheet, and the common halogenated benzene substructure of azole inhibitors was located deep in the same hydrophobic cavity. The results indicated that the dock results were in accord with SAR anal.

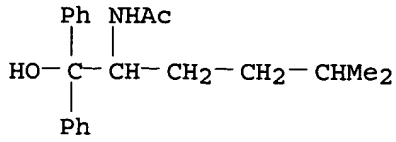
IT 136926-13-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(pharmacophoric conformations of azole antifungals and their interaction with active site of target enzyme)

RN 136926-13-1 CAPLUS
CN Benzamide, N-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

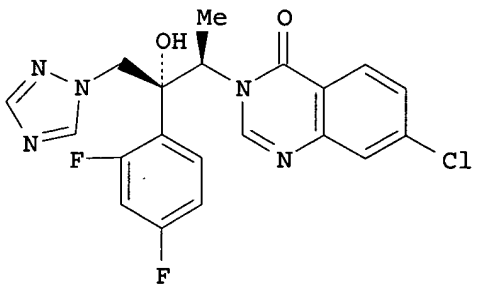


L19 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:79794 CAPLUS
DOCUMENT NUMBER: 130:227825
TITLE: Capillary electrochromatography as an alternative separation technique to high-performance liquid chromatography and capillary zone electrophoresis for the determination of drug related impurities in Lilly compound LY300164
AUTHOR(S): Reilly, John; Saeed, Mansoor
CORPORATE SOURCE: Lilly Research Centre, Eli Lilly and Company, Surrey, GU20 6PH, UK
SOURCE: Journal of Chromatography, A (1998), 829(1 + 2), 175-186
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Capillary electrochromog. (CEC) has been used to sep. pharmaceuticals from their related impurities; however, this has not been fully explored to date within the pharmaceutical industry. Generally capillary electrophoresis is used in either free-flow mode or in combination with micellar electrokinetic mode to complement the results obtained from the traditional method of HPLC. This paper explores the various separation modes now at hand in pharmaceutical labs. using a developmental Lilly compound LY300164 and its process impurities. Possible benefits and concerns for each of the separation modes are discussed by using the same sample and impurities to generate the results. Regulatory bodies prefer that purity assays for pharmaceuticals be complemented with another technique. This is to guarantee that no other hypothetical impurities which could potentially be present are seen in another technique. Traditionally, HPLC has been complemented with the use of TLC. This paper suggests that CEC can be used as a alternative purity assay for pharmaceuticals.
IT 221209-69-4
RL: ANT (Analyte); FMU (Formation, unclassified); ANST (Analytical study); FORM (Formation, nonpreparative)
(capillary electrochromatog. as alternative separation technique to HPLC and electrophoresis for determination of drug-related impurities)
RN 221209-69-4 CAPLUS
CN Acetamide, N-[1-(hydroxydiphenylmethyl)-4-methylpentyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:269995 CAPLUS
DOCUMENT NUMBER: 128:303693
TITLE: New Azole Antifungals. 3. Synthesis and Antifungal Activity of 3-Substituted-4(3H)-quinazolinones
AUTHOR(S): Bartroli, Javier; Turmo, Enric; Alguero, Monica; Boncompte, Eulalia; Vericat, Maria L.; Conte, Lourdes; Ramis, Joaquim; Merlos, Manuel; Garcia-Rafanell, Julian; Forn, Javier
CORPORATE SOURCE: Research Center, J. Uriach Cia. S.A., Barcelona, 08026, Spain
SOURCE: Journal of Medicinal Chemistry (1998), 41(11), 1869-1882
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A series of azole antifungal agents featuring a quinazolinone nucleus have been subjected to studies of structure-activity relationships. In general, these compds. displayed higher in vitro activities against filamentous fungi and shorter half-lives than the structures described in our preceding paper. The most potent products in vitro carried a halogen (or an isostere) at the 7-position of the quinazolinone ring. Using a murine model of systemic candidosis, oral activity was found to be dependent on hydrophobicity, which, in turn, modulated the compound's half-life. The 7-Cl derivative, (1R,2R)-7-chloro-3-[2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]quinazolin-4(3H)-one [I, UR-9825], was selected for further testing due to its high in vitro activity, low toxicity, good pharmacokinetic profile, and ease of obtention. Compound I is the (1R,2R) isomer of four possible stereoisomers. The other three isomers were also prepared and tested. The enantiomer (1S,2S) and the (1R,2S) epimer were inactive, whereas the (1S,2R) epimer retained some activity. In vitro, I was superior to fluconazole, itraconazole, SCH-42427, and TAK-187 and roughly similar to voriconazole and ER-30346. In vivo, I was only moderately active in a mouse model of systemic candidosis when administration was limited to the first day. This was attributed to its short half-life in that species (t1/2 = 1 h po). Protection levels comparable to or higher than those of

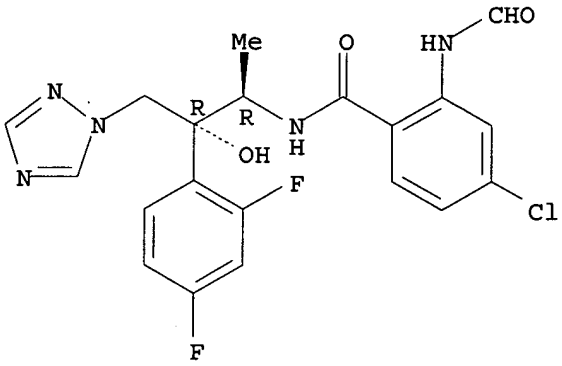
fluconazole, however, were observed in systemic candidosis models in rat and rabbit, where the half-life of the compound was found to be 6 and 9 h, resp. Finally, I showed excellent protection levels in an immunocompromised rat model of disseminated aspergillosis. The compound showed low toxicity signs when administered to rats at 250 mg/kg qd or at 100 mg/kg bid during 28 days.

IT 206350-06-3P 206350-07-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and antifungal activity of 3-substituted-4(3H)-quinazolinones)

RN 206350-06-3 CAPLUS

CN Benzamide, 4-chloro-N-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-2-(formylamino)- (9CI) (CA INDEX NAME)

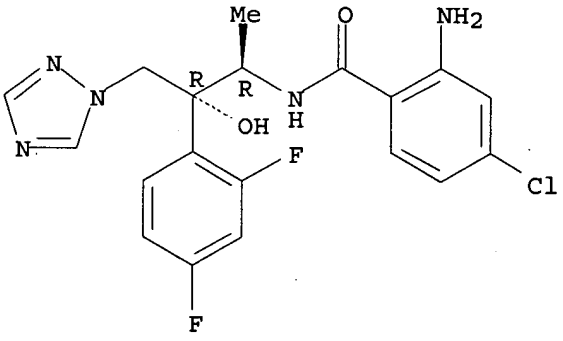
Absolute stereochemistry. Rotation (-).



RN 206350-07-4 CAPLUS .

CN Benzamide, 2-amino-4-chloro-N-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:488751 CAPLUS

DOCUMENT NUMBER: 125:142750

TITLE: Polyarylcarbamoylaza- and -carbamoylalkanedioic acids as squalene synthase inhibitors

INVENTOR(S): Pauls, Henry W.; Choi, Yong-Mi; Studt, Robert W.; Maguire, Martin P.; Spada, Alfred P.; Cha, Don D.

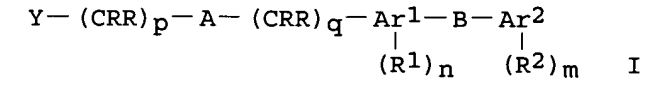
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer Pharmaceuticals Inc., USA

SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9618615	A1	19960620	WO 1995-US15364	19951129 <--
W: AL, AM, AT, AU, BB, BG, BR, BY, CA, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5556990	A	19960917	US 1994-357481	19941216 <--
CA 2207429	A1	19960620	CA 1995-2207429	19951129 <--
AU 9643698	A	19960703	AU 1996-43698	19951129 <--
AU 695852	B2	19980827		
EP 801644	A1	19971022	EP 1995-942489	19951129 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
JP 10511084	T	19981027	JP 1995-518973	19951129 <--

PRIORITY APPLN. INFO.: US 1994-357481 A 19941216
WO 1995-US15364 W 19951129

OTHER SOURCE(S): MARPAT 125:142750
GI



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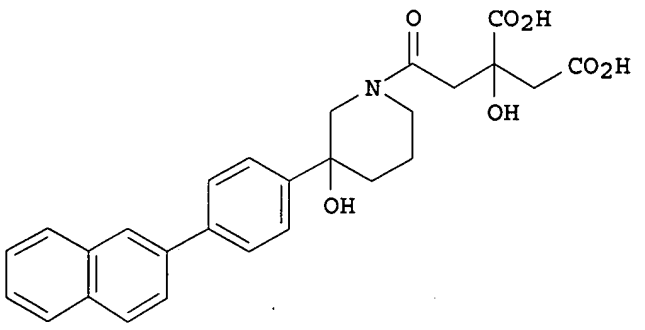


II

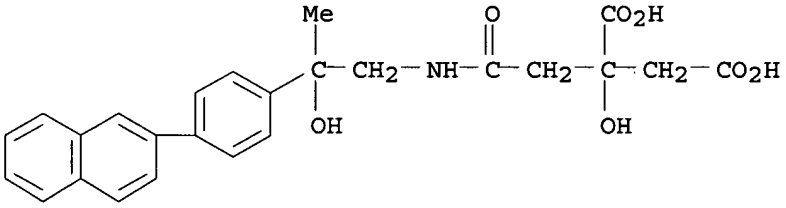
AB This invention relates to a class of novel dicarboxy amide derivs. of lipophilic amines I wherein: A is O, S, NR, SO, SO2, or a bond; B is (CRR)1-2, O, S, NR, SO, SO2, RC:CR, C.tplbond.C, CO, or a bond; Y is, e.g., RNZ(CRR)dCRR, N-Z-piperidyl, where Z is COWCR7[(CR3R4)fCO2R][(CR5R6)gCO2R]; W is a bond, (CRR)h, or NR; R = H, alkyl; R1, R2 are independently H, alkyl, alkoxy, OH, halo, haloalkyl, Ph; R3-R6 are independently H, alkyl; R7 is H, NRR, or OH and when W is (CRR)h then R7 is OH; one of R3-R7 is OH; Ar1 and Ar2 are independently a mono- or diaryl or heteroaryl; p and q are independently 0-3; p + q is 0-4; d is 0-3; p + q + d is 1-3; f is 0-2; g is 0-2; h is 1-2; m and n are independently 0-2; which exhibit squalene synthase inhibition properties. Compds. of this invention reduce levels of serum cholesterol in the body

without significantly reducing mevalonic metabolite synthesis. This invention relates also to pharmacol. compns. and method of treatment for lowering serum cholesterol levels using the compds. of this invention. Thus, e.g., coupling of prepared intermediates 3-hydroxy-3-(4-naphth-2-ylphenyl)piperidine with 3-hydroxy-3,4-bis(ethoxycarbonyl)butanoic acid afforded the diester intermediate which was hydrolyzed to the diaryl carbamoyl alkanedioic acid II which exhibited inhibition of squalene synthase with IC50 = 27 nM.

IT 179822-00-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(polyarylcarbamoylaza- and -carbamoylalkanedioic acids as squalene synthase inhibitors)

RN 179822-00-5 CAPLUS

CN Butanedioic acid, 2-hydroxy-2-[2-[[2-hydroxy-2-[4-(2-naphthalenyl)phenyl]propyl]amino]-2-oxoethyl]-, disodium salt (9CI) (CA INDEX NAME)

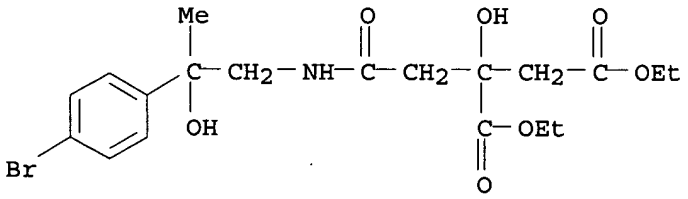


●2 Na

IT 179821-98-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(polyarylcarbamoylaza- and -carbamoylalkanedioic acids as squalene synthase inhibitors)

RN 179821-98-8 CAPLUS

CN Butanedioic acid, 2-[2-[[2-(4-bromophenyl)-2-hydroxypropyl]amino]-2-oxoethyl]-2-hydroxy-, diethyl ester (9CI) (CA INDEX NAME)



L19 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:655807 CAPLUS

DOCUMENT NUMBER: 121:255807

TITLE: N-[(hydroxy)(triazolyl)propyl] amides as novel orally active antifungal agents.

INVENTOR(S): Bartroli, Javier; Turmo, Enric Dr; Turmo, Enric; Almansa, Carmen

PATENT ASSIGNEE(S): J. Uriach y Cia. S.A., Spain

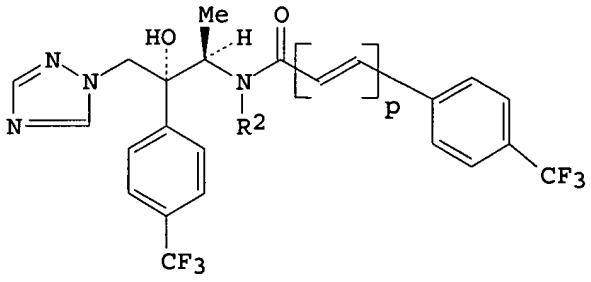
SOURCE: Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 612734	A1	19940831	EP 1994-102139	19940211 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
ES 2099004	A1	19970501	ES 1993-268	19930211 <--
ES 2099004	B1	19980116		
CA 2113972	A1	19940812	CA 1994-2113972	19940121 <--
JP 06271551	A	19940927	JP 1994-39178	19940214 <--

PRIORITY APPLN. INFO.: ES 1993-268 A 19930211
OTHER SOURCE(S): MARPAT 121:255807
GI



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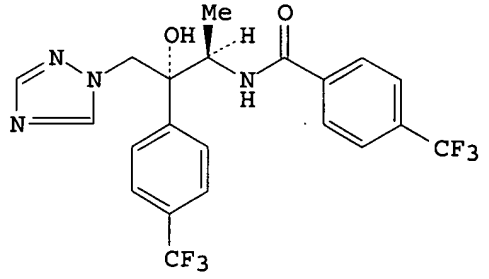


II

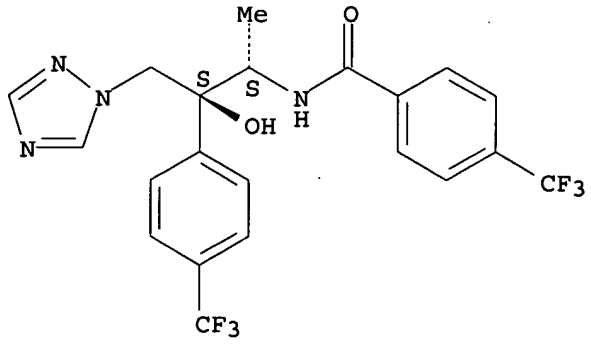
AB Orally active antifungal agents, N-[(hydroxy)(triazolyl)propyl] amides I (R1 = H; R2 = H, alkyl; R1R2 together = CH2; p = 0-1) were disclosed. An example compound, 3-[4-(trifluoromethyl)benzoylamino]-2-[4-(trifluoromethyl)phenyl]-1-(1H-1,2,4-triazol-1-yl)-2-butanol (II) was prepared Pharmacol. test data were not shown.

IT 158558-34-0P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(N-[(hydroxy)(triazolyl)propyl] amides as fungicides)

RN 158558-34-0 CAPLUS

CN Benzamide, N-[2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)-2-[4-(trifluoromethyl)phenyl]propyl]-4-(trifluoromethyl)-, (R*,R*)- (9CI) (CA INDEX NAME)

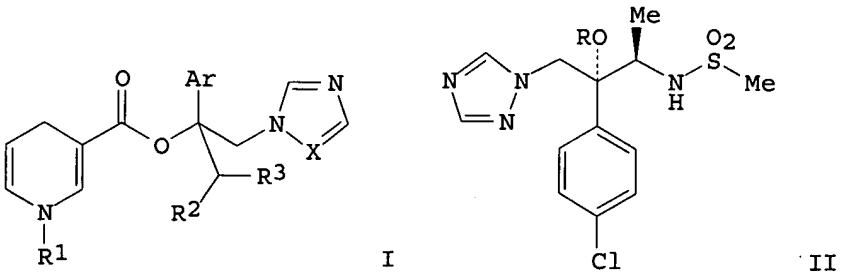
Relative stereochemistry.



L19 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:298630 CAPLUS
DOCUMENT NUMBER: 120:298630
TITLE: Process for the preparation of new dihydropyridine prodrugs of triazole and imidazole antifungal agents
INVENTOR(S): Bertroli, Javier; Belloc, Jordi; Carceller, Elena; Almansa, Carmen
PATENT ASSIGNEE(S): J. Uriach y Cia. S.A., Spain
SOURCE: Span., 16 pp.
CODEN: SPXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 2040181	A1	19931001	ES 1992-754	19920330 <--
ES 2040181	B1	19940516		

PRIORITY APPLN. INFO.: ES 1992-754 19920330
OTHER SOURCE(S): MARPAT 120:298630
GI



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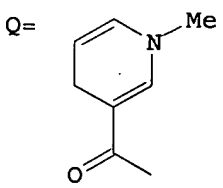
II



AB Title esters I [X = N, CH; R1 = alkyl, benzyl; R2 = H, alkyl; R3 = 1,2,4-triazol-1-yl, SO2Me, NHCOR4, NHCO2R4, NR5SO2R4; R4 = (cyclo)alkyl,

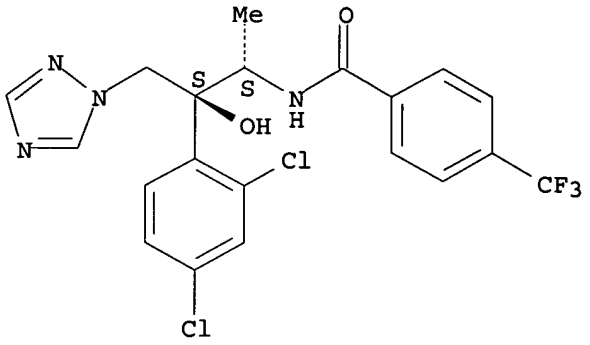
haloalkyl, (un)substituted Ph, naphthyl, (iso)quinolyl, 5- or 6-membered (un)substituted heterocyclyl; R5 = H, (cyclo)alkyl, haloalkyl, cycloalkylmethyl, (un)substituted phenylalkyl, heterocyclylalkyl, (un)substituted Ph or heterocyclyl, naphthyl, etc.; Ar = Ph (un)substituted by halo and/or CF3] were prepared by O-acylation of corresponding azole alcs. with nicotinic acid derivs., quaternization of the pyridine nucleus in the products, and reduction to the dihydropyridines by an agent such as Na dithionite. I are antifungal prodrugs (no data), designed for treatment of central nervous system infections, and particularly cryptococcic meningitis accompanying AIDS. For example, the known (R*,R*)-diastereomer of alc. II (R = H) underwent esterification with nicotinoyl chloride-HCl (89%), followed by N-methylation of the resultant II (R = 3-pyridinylcarbonyl) with MeI in Me2CO (74%), and reduction by Na2S2O4 and NaHCO3 in a deoxygenated mixture of EtOAc and H2O, to give 79% title compound II (R = Q).

IT 126916-55-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification with nicotinoyl chloride, in preparation of dihydropyridine-based antifungal prodrug)

RN 126916-55-0 CAPLUS

CN Benzamide, N-[2-(2,4-dichlorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-4-(trifluoromethyl)-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L19 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1986:430050 CAPLUS

DOCUMENT NUMBER: 105:30050

TITLE: Benzothiophenes, compositions containing them and their use

INVENTOR(S): Tischler, Allan N.; Durette, Philippe L.; Witzel, Bruce E.; Rupprecht, Kathleen M.; Gallagher, Timothy F.; Goldenberg, Marvin M.; Allison, Debra L.

PATENT ASSIGNEE(S): Merck and Co., Inc. , USA

SOURCE: Eur. Pat. Appl., 79 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

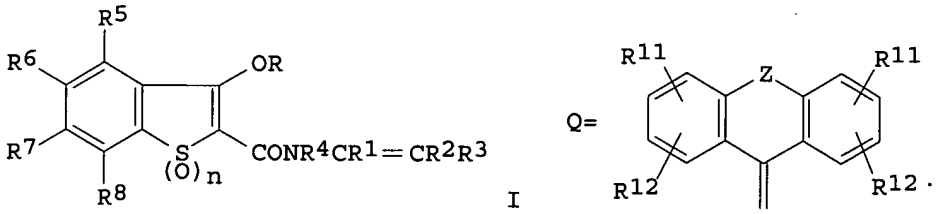
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 160408	A1	19851106	EP 1985-302275	19850401 <--
EP 160408	B1	19890823		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4760086	A	19880726	US 1985-705115	19850227 <--
CA 1298837	C	19920414	CA 1985-477848	19850328 <--
ES 541781	A1	19870501	ES 1985-541781	19850329 <--

DK 8501455	A	19851003	DK 1985-1455		19850401 <--
AU 8540564	A	19851010	AU 1985-40564		19850401 <--
AU 572637	B2	19880512			
ZA 8502439	A	19860430	ZA 1985-2439		19850401 <--
JP 60226875	A	19851112	JP 1985-68589		19850402 <--
JP 03014826	B	19910227			
CN 85107805	A	19861231	CN 1985-107805		19851011 <--
ES 550966	A1	19871116	ES 1986-550966		19860116 <--
US 5068248	A	19911126	US 1989-369982		19890622 <--
PRIORITY APPLN. INFO.:			US 1984-596134	A	19840402
			US 1985-705115	A	19850227
			US 1988-172538	B2	19880324

OTHER SOURCE(S): MARPAT 105:30050

GI



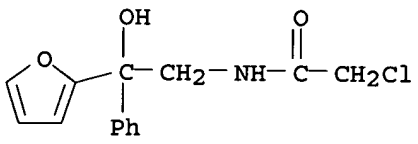
I

AB Benzothiophenes I [R = R9, COR9, CO2R9, CONR9R10, COSR9, (CH2)mCOR9, (CH2)mOR9, (CH2)mO2COR9, (CH2)mNR9R10, (CH2)mNR9COR10; R1-R3 = halo, R; CR2R3 = Q; R4 = R, CR1:CR2R3; R5-R8 = R, R11; R9, R10 = H, alkyl, alkenyl, alkynyl, cycloalkyl, haloalkyl, (un)substituted aryl, heteroaryl, PhCH2, phenylalkenyl, phenylalkynyl; R11, R12 = halo, alkenyl, alkynyl, cyano, NO2, R13, SR13, OR13, COR13, CO2R13, SOR13, SO2R13, CF2SR13, etc.; R13= H, alkyl, haloalkyl, naphthyl, (un)substituted Ph; Z = (CH2)x, O, S, SO, SO2, (un)substituted NH; m = 1, 2; n, x = 0-2] were prepared I are effective inhibitors of both cyclooxygenase and lipoxygenase and, thus, are useful in the treatment of pain, fever, inflammation, asthma, allergy, glaucoma, psoriasis and other prostaglandin- and/or leukotriene-mediated diseases. I also exhibit cytoprotective activity which does not involve gastric acid-secretion inhibition. Thus, Me 5-fluorosalicylate was esterified with Me2NCSCl to give 53% O-(2-carbomethoxy-4-fluorophenyl) dimethylthiocarbamoate, which was isomerized by heating at 240° to give 53.5% S-ester. This ester was treated with NaOMe and then ClCH2CONH2 to give 73% 5-fluoro-3-hydroxybenzo[b]thiophene-2-carboxamide, which was N-alkenylated with Ph2CHCO to give 82% I (R = R1 = R4 = R5 = R7 = R8 = H, R2 = R3 = Ph, R6 = F). I (5 mg) was aseptically combined with 995 mg petrolatum to give an ophthalmic ointment.

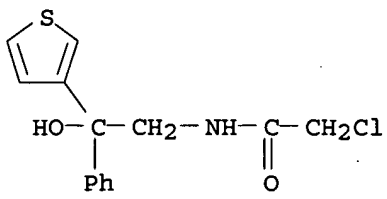
IT 102565-26-4 102565-27-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization reaction of, with (trifluoromethyl)thiosalicylate)

RN 102565-26-4 CAPLUS

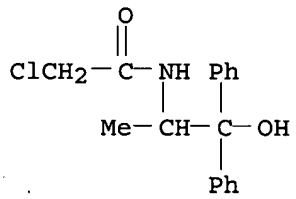
CN Acetamide, 2-chloro-N-[2-(2-furanyl)-2-hydroxy-2-phenylethyl]- (9CI) (CA INDEX NAME)



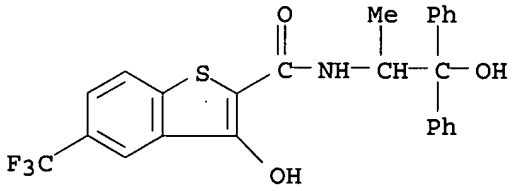
RN 102565-27-5 CAPLUS
CN Acetamide, 2-chloro-N-[2-hydroxy-2-phenyl-2-(3-thienyl)ethyl]- (9CI) (CA INDEX NAME)



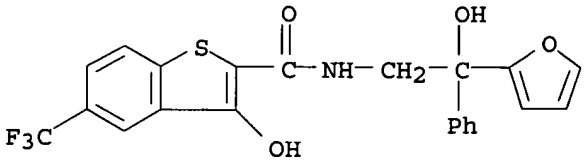
IT 5197-13-7P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization reaction of, with (trifluoromethyl)thiosalicylate)
RN 5197-13-7 CAPLUS
CN Acetamide, 2-chloro-N-(2-hydroxy-1-methyl-2,2-diphenylethyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 102565-21-9P 102565-24-2P 102565-25-3P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of)
RN 102565-21-9 CAPLUS
CN Benzo[b]thiophene-2-carboxamide, 3-hydroxy-N-(2-hydroxy-1-methyl-2,2-diphenylethyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

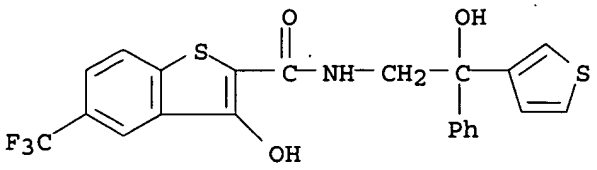


RN 102565-24-2 CAPLUS
CN Benzo[b]thiophene-2-carboxamide, N-[2-(2-furanyl)-2-hydroxy-2-phenylethyl]-3-hydroxy-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 102565-25-3 CAPLUS
CN Benzo[b]thiophene-2-carboxamide, 3-hydroxy-N-[2-hydroxy-2-phenyl-2-(3-

thienyl)ethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

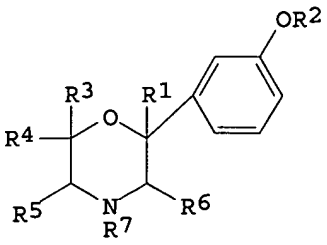


L19 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:569197 CAPLUS
DOCUMENT NUMBER: 95:169197
TITLE: Morpholine derivatives, their use and pharmaceutical compositions containing them
INVENTOR(S): White, Alan Chapman; Edington, Edwin Trevor
PATENT ASSIGNEE(S): John Wyeth and Brother Ltd., UK
SOURCE: Eur. Pat. Appl., 43 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 27695	A1	19810429	EP 1980-303473	19801002 <--
EP 27695	B1	19831012		
R: AT, BE, CH, DE, FR, IT, LU, NL, SE				
ZA 8006017	A	19820428	ZA 1980-6017	19800929 <--
CA 1126731	A1	19820629	CA 1980-361904	19801001 <--
AU 8062922	A	19810430	AU 1980-62922	19801002 <--
AU 531586	B2	19830901		
GB 2061272	A	19810513	GB 1980-31816	19801002 <--
GB 2061272	B	19830810		
AT 4980	T	19831015	AT 1980-303473	19801002 <--
US 4360519	A	19821123	US 1980-193779	19801003 <--
DK 8004410	A	19810421	DK 1980-4410	19801017 <--
DK 151800	B	19880104		
DK 151800	C	19880606		
FI 8003277	A	19810421	FI 1980-3277	19801017 <--
JP 56065880	A	19810603	JP 1980-145564	19801017 <--
ES 496074	A1	19811001	ES 1980-496074	19801018 <--

PRIORITY APPLN. INFO.: GB 1979-36502 A 19791020
EP 1980-303473 A 19801002

OTHER SOURCE(S): MARPAT 95:169197
GI



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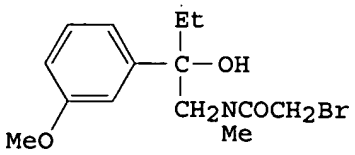


II

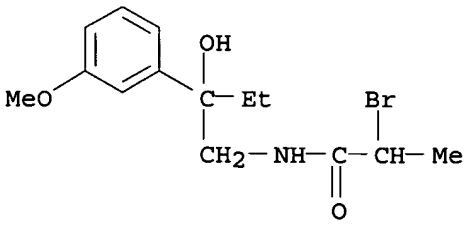
AB Morpholines I (R1 = alkyl, R2 = H, alkyl, benzyl, alkoxymethyl, acyl; R3 =

H, alkyl, Ph; R4, R5, R6 = H, alkyl; R7 = H, alkyl, alkenyl, alkynyl), possessing analgesic and narcotic antagonistic activities, were prepared Thus, cyclization of II followed by LiAlH4 reduction and demethylation gave I (R1 = Et, R2-R6 = H, R7 = Me). I (R1 = Et, R2, R3, R5, R6 = H, R4 = R7 = Me) at 25 mg/kg had analgesic activity in rat tail flick test and had a s.c. ED50 of 1.9 mg/kg in narcotic antagonist test.

IT 79290-91-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 79290-91-8 CAPLUS

CN Propanamide, 2-bromo-N-[2-hydroxy-2-(3-methoxyphenyl)butyl]- (9CI) (CA INDEX NAME)



L19 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1950:3119 CAPLUS

DOCUMENT NUMBER: 44:3119

ORIGINAL REFERENCE NO.: 44:633a-h

TITLE: Synthesis of isoquinoline derivatives

AUTHOR(S): Whaley, Wilson M.; Hartung, Walter H.

SOURCE: Journal of Organic Chemistry (1949), 14, 650-4
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 44:3119

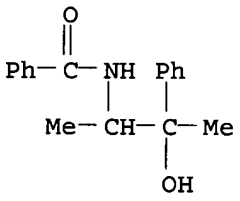
AB The reactions of Bischler and Napieralski (Ber. 26, 1903(1893)) and Pictet and Gams (C.A. 3, 2958) have been applied to the synthesis of isoquinolines (I) and 3,4-dihydroisoquinolines (II) alkylated in positions 3 and 4 but unsubstituted in the benzenoid ring, to yield compds. of potential pharmacol. interest and to explore the effects of substitution in the ethylamine side chain. The preparation of I from N-acyl-2-hydroxyphenethylamines required more drastic conditions than the preparation of the corresponding II, but the yields were not lower. Synthesis of I or II having alkyl groups in the 3-position was possible only in low yield, the yield decreasing with increase in the size of the alkyl group. II alkylated in the 4-position were easier to prepare than the corresponding I. In the 1- or 3-position a Ph group was less hindering than an alkyl group of comparable size. The following compds., prepared from the 1-phenyl-2-amino-1-alkanols prepared by the methods of Hartung and Munch (C.A. 23, 3912; 26, 118) by treating the amine in EtOH-free Et2O with 1 equivalent each of 20% NaOH and the appropriate acid chloride, or by treating the amine-HCl in EtOH-free Et2O with 2 equivs. of 20% NaOH and 1 equivalent of the acid chloride, are described (yield and m.p. given): 1-Phenyl-2-butyrylamino-1-propanol, 79%, 93-4°; 1-phenyl-2-(phenylacetamido)-1-propanol, 78%, 117-19°; 1-phenyl-2-benzamido-1-butanol, 98%, 156-7°; 2-phenyl-3-benzamido-2-butanol, 81%, 150-1°; 1-phenyl-2-benzamido-1-pentanol, 95%, 150-1°; 1-phenyl-2-benzamido-1-hexanol, 74%, 151-2°; 1-phenyl-2-benzamido-1-octanol, 86%, 77-8°; 1-(1-naphthyl)-2-benzamido-1-propanol, 83%, 172-3°. Numerous techniques were employed in the preparation of the I derivs. The following are recommended as

generally useful methods. To prepare II, the amide is refluxed with 2 parts each of P2O5 and POCl3 in 15 parts dry xylene 1 h. under anhydrous conditions. To prepare I, the amide is refluxed with 5 parts P2O5 and 10 parts POCl3 in 25 parts dry xylene 3 h. under anhydrous conditions. At the end of the refluxing time, the excess dehydrating agents are hydrolyzed with ice, the layers separated, the aqueous layer washed with C6H6, then made strongly alkaline with 20% NaOH, the desired base extracted with C6H6, and the extract dried over MgSO4 and treated with HCl; there usually seps. an oily HCl derivative which may be recrystd. from iso-PrOH-ligroin after evaporation of
the C6H6. The compds. prepared are listed in the order of substituent, yield, m.p. of picrate, m.p. of HCl salt. 3,4-Dihydroisoquinolines: 1-Me, 70%, 193°, 196-8°; 1-Ph, 100%, 178°, 245-8°; 1-benzyl, 80%, 176-8°, 227-9°; 1-phenyl-3-Me, 24%, -, 205-10°; 1-phenyl-4-Me, 92%, 152°, 193°. Isoquinolines: 1-Ph, 91%, 174°, 237-9°; 1,3-di-Me, 37%, -, 168°; 1-propyl-3-Me, 35%, -, 165°; 1-phenyl-3-Me, 50% (free base, m. 123-5°), 188°, 229°; 1-benzyl-3-Me, 20%,-, 207° (decomposition); 1-phenyl-3-Et, 26%, -, 210°; 1-phenyl-4-Et, 10%, 165°, 113-15°; 1-phenyl-3-Pr, 20%, -, 180-90°; 1-phenyl-3-Bu, 1%, -, approx. 130°; 1,3-di-Ph, 20%, 185°, approx. 185°; 1-phenyl-3-methyl-5,6-dibenzyl, 12%, -, 235° (decomposition).

IT 860683-96-1P, Benzamide, N-(β-hydroxy-α,β-dimethylphenethyl)-
RL: PREP (Preparation)
(preparation of)

RN 860683-96-1 CAPLUS

CN Benzamide, N-(β-hydroxy-α,β-dimethylphenethyl)- (5CI) (CA INDEX NAME)



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L18            0 S L16 AND PHARMACEUTICALLY
L19           11 S L16 AND PHARMA?
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